

ON THE EXTREMA OF A NONCONVEX FUNCTIONAL WITH DOUBLE-WELL POTENTIAL IN HIGHER DIMENSIONS

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ABSTRACT. This paper mainly addresses the extrema of a nonconvex functional with double-well potential in higher dimensions through the approach of nonlinear partial differential equations. Based on the canonical duality method, the corresponding Euler–Lagrange equation with Neumann boundary condition can be converted into a cubic dual algebraic equation, which will help find the local extrema for the primal problem. In comparison with the 1D case discussed by D. Gao and R. Ogden, there exists huge difference in higher dimensions, which will be explained in the theorem.

RÉSUMÉ. Dans cet article, on considère essentiellement les extrema d'un fonctionnel nonconvexe avec double puits de potentiel dans les dimensions supérieures. En appliquant la méthode de dualité canonique, l'équation aux dérivées partielles (EDPs) nonlinéaire, c'est-à-dire, l'équation d'Euler–Lagrange avec les conditions aux limites de Neumann, peut être convertie en un dual algébrique cubique, qui nous aidera à démontrer le principe du minimum (ou du maximum) local pour le problème primal. En comparaison avec le cas 1D étudié par D. Gao et R. Ogden, il existe énorme différence dans les dimensions supérieures, et on l'expliquera dans le théorème.

1. INTRODUCTION

The double-well potential was first studied by Van der Waals in the nineteenth century for a compressible fluid whose free energy at a constant temperature depends on both the density and the density gradient [17]. Afterwards, lots of applications of this nonconvex function have been found in nonlinear sciences, i.e., in phase transitions of Ericksen's bar [5], or the mathematical theory of super-conductivity [11], etc. In this paper, we consider the fourth-order polynomial defined by

$$H(|\vec{\gamma}|) := \nu/2 \left(1/2 |\vec{\gamma}|^2 - \lambda \right)^2, \quad \vec{\gamma} \in \mathbb{R}^n, \quad \nu, \lambda > 0 \text{ are constants, } |\vec{\gamma}|^2 = \vec{\gamma} \cdot \vec{\gamma}.$$

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In quantum mechanics, if $\vec{\gamma}$ represents Higgs' field strength, then $H(|\vec{\gamma}|)$ is the Higgs' potential [13]. It was discovered in the context of post-buckling analysis [6] that the stored potential energy of a large deformed beam model in 1D is exactly a double-well function, where each potential well represents a possible buckled beam state, and the local maximizer is corresponding to the unbuckled state [8]. As a matter of fact, the polynomial is also the well-known Landau's second-order free energy, each of its local minimizers represents a possible phase state of the material, while each local maximizer characterizes the critical conditions that lead to the phase transitions etc. [10, 11].

The purpose of this paper is to find the extrema of the following nonconvex total potential energy functional in higher dimensions,

$$(1) \quad I[u] := \int_{\Omega} \left(H(|\nabla u|) - fu \right) dx,$$

where $\Omega = \text{Int}\left\{ \mathbb{B}(O, R_1) \setminus \mathbb{B}(O, R_2) \right\}$, $R_1 > R_2 > 0$, $\mathbb{B}(O, R_1)$ and $\mathbb{B}(O, R_2)$ denote two open balls with center O and radii R_1 and R_2 in the Euclidean space \mathbb{R}^n , respectively. "Int" denotes the interior points. In addition, let $\Sigma_1 := \{x : |x| = R_1\}$, and $\Sigma_2 := \{x : |x| = R_2\}$, then the boundary $\partial\Omega = \Sigma_1 \cup \Sigma_2$. The radially symmetric function $f \in C(\overline{\Omega})$ satisfies the normalized balance condition

$$(2) \quad \int_{\Omega} f(|x|) dx = 0,$$

and

$$(3) \quad f(|x|) = 0 \text{ if and only if } |x| = R_3 \in (R_2, R_1).$$

Moreover, its L^1 -norm is sufficiently small such that

$$(4) \quad \|f\|_{L^1(\Omega)} < 4\lambda\nu R_2^{n-1} \sqrt{2\lambda\pi^n} / (3\sqrt{3}\Gamma(n/2)),$$

where Γ stands for the Gamma function. This assumption is reasonable since large $\|f\|_{L^1(\Omega)}$ may possibly lead to instant fracture. The deformation u is subject to the following three constraints,

$$(5) \quad u \text{ is radially symmetric on } \overline{\Omega},$$

$$(6) \quad u \in W^{1,\infty}(\Omega) \cap C(\overline{\Omega}),$$

$$(7) \quad \nabla u \cdot \vec{n} = 0 \text{ on both } \Sigma_1 \text{ and } \Sigma_2,$$

where \vec{n} denotes the unit outward normal on $\partial\Omega$.

By variational calculus, one derives a correspondingly nonlinear Euler–Lagrange equation for the primal nonconvex functional, namely,

$$(8) \quad \text{div}\left(\nabla H(|\nabla u|)\right) + f = 0 \text{ in } \Omega,$$

equipped with the Neumann boundary condition (7). Clearly, (8) is a highly nonlinear partial differential equation which is difficult to solve by the direct approach or numerical method [2, 15]. However, by the canonical duality method, one is able to

demonstrate the existence of solutions for this type of equations.

This paper is aimed to solve the challenging nonconvex variational problem by using the *canonical duality theory*, which can be applied in solving a large class of nonconvex/nonsmooth/discrete problems in multidisciplinary fields including mathematical physics, global optimization, computational science, etc. For instance, Gao and Ogden have introduced this method to the 1D problems in finite deformation mechanics [9] and phase transitions of the Ericksen's bar [10]. Their work showed that the nonlinear differential equations can be converted into dual algebraic equations and help us find the possible nonsmooth solutions.

Before introducing the main result, we denote

$$F(r) := -1/r^n \int_{R_2}^r f(\rho) \rho^{n-1} d\rho, \quad r \in [R_2, R_1].$$

Next, we define a polynomial of third order as follows,

$$E(y) := 2y^2(\lambda + y/\nu), \quad y \in [-\nu\lambda, +\infty).$$

Furthermore, for any $A \in [0, 8\lambda^3\nu^2/27)$,

$$E_3^{-1}(A) \leq E_2^{-1}(A) \leq E_1^{-1}(A)$$

stand for the three real-valued roots for the equation $E(y) = A$.

At the moment, we would like to introduce the theorem of multiple extrema for the nonconvex functional (2).

Theorem 1.1. *For any radially symmetric function $f \in C(\overline{\Omega})$ satisfying (2)–(4), we have three solutions for the nonlinear Euler–Lagrange equation (8) equipped with the Neumann boundary condition, namely*

- For any $r \in [R_2, R_1]$, \bar{u}_1 defined below is a local minimizer for the nonconvex functional (2).

$$(9) \quad \bar{u}_1(|x|) = \bar{u}_1(r) := \int_{R_2}^r F(\rho) \rho / E_1^{-1}(F^2(\rho) \rho^2) d\rho + C_1, \quad \forall C_1 \in \mathbb{R}.$$

- For any $r \in [R_2, R_1]$, \bar{u}_2 defined below is a local minimizer for the nonconvex functional (2) in 1D. While for the higher dimensions $n \geq 2$, \bar{u}_2 is not necessarily a local minimizer for (2) in comparison with the 1D case.

$$(10) \quad \bar{u}_2(|x|) = \bar{u}_2(r) := \int_{R_2}^r F(\rho) \rho / E_2^{-1}(F^2(\rho) \rho^2) d\rho + C_2, \quad \forall C_2 \in \mathbb{R}.$$

- For any $r \in [R_2, R_1]$, \bar{u}_3 defined below is a local maximizer for the nonconvex functional (2).

$$(11) \quad \bar{u}_3(|x|) = \bar{u}_3(r) := \int_{R_2}^r F(\rho) \rho / E_3^{-1}(F^2(\rho) \rho^2) d\rho + C_3, \quad \forall C_3 \in \mathbb{R}.$$

Remark 1.2. *From the above theorem, one knows, it is incorrect to simply generalize the 1D case discussed in [10] to higher dimensions. Each of these solutions is a critical point of I , i.e., it could be either an extremum or a saddle point of the total potential. This phenomenon has been verified by Ericksen who proved that many local solutions are metastable and may have arbitrary number of phase interfaces.*

Remark 1.3. *Compared with convex problems, a fundamentally different issue in nonconvex analysis is that the solutions of the boundary-value problem is not equivalent to the associated minimum variational problem and it is extremely difficult to use traditional direct approaches in solving the nonconvex variational problems. In particular, it is discovered that for certain given external loads, a global or local minimizer is nonsmooth and cannot be determined by any Newton-type numerical methods.*

The rest of the paper is organized as follows. In Section 2, first we introduce some useful notations which will simplify our proof considerably. Then, we apply the canonical dual transformation to deduce a perfect dual problem corresponding to the primal nonconvex variational problem and a pure complementary energy principle. In the final analysis, we apply the canonical duality theory to prove Theorem 1.1.

2. PROOF OF THE MAIN RESULT

2.1. Some useful notations.

- $\vec{\sigma}$ is the Gâteaux derivative of H given by

$$\vec{\sigma}(x) = (\sigma^{(1)}(x), \dots, \sigma^{(n)}(x)) = \nu(1/2|\nabla u|^2 - \lambda)\nabla u.$$

From the physician' viewpoint, if ∇u represents a deformation gradient, then the vector $\vec{\sigma}$ is the so-called first Piola-Kirchhoff stress in the finite deformation theory.

- Φ is a nonlinear geometric mapping defined as

$$\Phi(u) := 1/2|\nabla u|^2.$$

For convenience's sake, denote $\xi := \Phi(u)$. It is evident that ξ belongs to the function space \mathcal{U} given by

$$\mathcal{U} := \left\{ \phi \in L^\infty(\Omega) \mid \phi \geq 0 \right\}.$$

- Ψ is a canonical energy defined as

$$\Psi(\xi) := \nu/2(\xi - \lambda)^2,$$

which is a convex function with respect to ξ . For simplicity, denote $\zeta := \nu(\xi - \lambda)$, which is the Gâteaux derivative of Ψ with respect to ξ . Moreover, ζ is invertible with respect to ξ and belongs to the function space \mathcal{V} ,

$$\mathcal{V} := \left\{ \phi \in L^\infty(U) \mid \phi \geq -\nu\lambda \right\}.$$

- Ψ_* is defined as

$$\Psi_*(\zeta) := \xi\zeta - \Psi(\xi) = \zeta^2/(2\nu) + \lambda\zeta.$$

2.2. Canonical duality techniques.

Definition 2.1. By Legendre transformation, one defines a Gao–Strang total complementary energy functional Ξ ,

$$\Xi(u, \zeta) := \int_{\Omega} \left\{ \Phi(u)\zeta - \Psi_*(\zeta) - fu \right\} dx.$$

Next we introduce an important *criticality criterium* for the Gao–Strang total complementary energy functional.

Definition 2.2. $(\bar{u}, \bar{\zeta})$ is called a critical pair of Ξ if and only if

$$(12) \quad D_u \Xi(\bar{u}, \bar{\zeta}) = 0,$$

$$(13) \quad D_{\zeta} \Xi(\bar{u}, \bar{\zeta}) = 0,$$

where D_u, D_{ζ} denote the partial Gâteaux derivatives of Ξ , respectively.

Indeed, by variational calculus, one has the following observation from (12) and (13).

Lemma 2.3. On the one hand, for any fixed $\zeta \in \mathcal{V}$, (12) is equivalent to the equilibrium equation

$$\operatorname{div}(\zeta \nabla \bar{u}) + f = 0 \quad \text{in } \Omega,$$

with the Neumann boundary condition. On the other hand, for any fixed u subject to (5)–(7), (13) is consistent with the notations before,

$$\Phi(u) = D_{\zeta} \Psi_*(\bar{\zeta}).$$

Lemma 2.3 indicates that \bar{u} from the critical pair $(\bar{u}, \bar{\zeta})$ solves the Euler–Lagrange equation (8).

Definition 2.4. From Definition 2.1, one defines the Gao–Strang pure complementary energy I_d in the form

$$I_d[\zeta] := \Xi(\bar{u}, \zeta),$$

where \bar{u} solves the Euler–Lagrange equation (8).

To simplify the discussion, one uses another representation of the pure energy I_d given by the following lemma through integrating by parts.

Lemma 2.5. The pure complementary energy functional I_d can be rewritten as

$$(14) \quad I_d[\zeta] = -1/2 \int_{\Omega} \left\{ |\vec{\sigma}|^2 / \zeta + 2\lambda\zeta + \zeta^2 / \nu \right\} dx,$$

where $\vec{\sigma}$ satisfies

$$(15) \quad \operatorname{div} \vec{\sigma} + f = 0 \quad \text{in } \Omega,$$

equipped with $\vec{\sigma} \cdot \vec{n} = 0$ on $\partial\Omega$.

With the above discussion, indeed, by calculating the Gâteaux derivative of I_d with respect to ζ , one has

Lemma 2.6. *The variation of I_d with respect to ζ leads to the cubic dual algebraic equation (DAE), namely*

$$(16) \quad |\vec{\sigma}|^2 = 2\bar{\zeta}^2(\lambda + \bar{\zeta}/\nu),$$

where $\bar{\zeta}$ is from the critical pair $(\bar{u}, \bar{\zeta})$.

Remark 2.7. *From (16), it is easy to check that $|\vec{\sigma}|^2$ has a maximum $8\lambda^3\nu^2/27$ at $\bar{\zeta} = -2\lambda\nu/3$ and a minimum 0 at $\bar{\zeta} = 0$.*

- *If $|\vec{\sigma}|^2 = 8\lambda^3\nu^2/27$, then there exist two real roots.*
- *If $|\vec{\sigma}|^2 \in (8\lambda^3\nu^2/27, \infty)$, then there exists only one positive real root.*
- *If $|\vec{\sigma}|^2 \in [0, 8\lambda^3\nu^2/27)$, then there exist three real roots listed below,*

$$(17) \quad \bar{\zeta}_1 > 0 > \bar{\zeta}_2 > -2\nu\lambda/3 > \bar{\zeta}_3 > -\nu\lambda.$$

- *For $|\vec{\sigma}|^2 = 0$, there also exist three real roots such as*

$$(18) \quad \bar{\zeta}_1 = \bar{\zeta}_2 = 0, \quad \bar{\zeta}_3 = -\nu\lambda.$$

2.3. Proof of Theorem 1.1. Actually, a radially symmetric solution for the Euler–Lagrange equation (8) is of the form

$$\vec{\sigma} = F(r)(x_1, \dots, x_n) = F\left(\sqrt{\sum_{i=1}^n x_i^2}\right)(x_1, \dots, x_n),$$

where F is the unique solution for the nonhomogeneous linear differential equation

$$F'(r) + nF(r)/r = -f(r)/r, \quad r \in [R_2, R_1].$$

with $F(R_2) = 0$. Furthermore, the normalized balance condition (2) assures that $F(R_1) = 0$, which indicates $\vec{\sigma} \cdot \vec{n} = 0$ on $\partial\Omega$.

From the above discussion, one deduces that once $\vec{\sigma}$ is given, then an analytic solution of the Euler–Lagrange equation (8) can be presented as

$$(19) \quad \bar{u}_i(|x|) = \int_{x_0}^x \vec{\eta}_i \vec{dt},$$

where $x \in \bar{\Omega}$, $x_0 \in \partial\Omega$, $\vec{\eta}_i = (\eta_i^{(1)}, \eta_i^{(2)}, \dots, \eta_i^{(n)}) := \vec{\sigma}/\bar{\zeta}_i$, which satisfies the condition for path independent integrals, namely, for $i = 1, 2, 3$,

$$\partial_{x_j} \eta_i^{(k)} - \partial_{x_k} \eta_i^{(j)} = 0, \quad j, k = 1, \dots, n.$$

By direct calculation for I and I_d , respectively, it is easy to check that the pure complementary energy functional I_d is perfectly dual to the total potential energy functional I , and the identities

$$I[\bar{u}_i] = I_d[\bar{\zeta}_i], \quad i = 1, 2, 3$$

indicate there is no duality gap between the primal and dual variational problems.

Next, we prove the local extrema. On the one hand, for any test function $\phi \in W^{1,\infty}(\Omega)$, the second variational form $\delta_\phi^2 I$ is equal to

$$(20) \quad \nu \int_{\Omega} \left\{ |\nabla \bar{u} \cdot \nabla \phi|^2 + \left(1/2 |\nabla \bar{u}|^2 - \lambda \right) |\nabla \phi|^2 \right\} dx.$$

On the other hand, for any test function $\psi \in \mathcal{V}$, the second variational form $\delta_\psi^2 I_d$ is equal to

$$(21) \quad - \int_{\Omega} \left\{ |\vec{\sigma}|^2 / \bar{\zeta}^3 + 1/\nu \right\} \psi^2 dx.$$

Actually, (3) and (4) indicate $0 < F^2(r)r^2 < 8\lambda^3\nu^2/27$ for any $r \in (R_2, R_1)$. Indeed, let

$$G(r) := \int_{R_2}^r f(\rho) \rho^{n-1} d\rho.$$

Its derivative is $G'(r) = f(r)r^{n-1}$ and $G(R_2) = G(R_1) = 0$. From (3), since $f(|x|) = 0$ if and only if $|x| = R_3 \in (R_2, R_1)$, without loss of generality, we assume that

$$f(r) = \begin{cases} > 0, & r \in [R_2, R_3); \\ < 0, & r \in (R_3, R_1]. \end{cases}$$

From the above assumption and the fact $G(R_2) = G(R_1) = 0$, one has $G(r) > 0$, $r \in (R_2, R_1)$. As a result, $F(r)$ does not change its sign in (R_2, R_1) and

$$F^2(r)r^2 = r^{2-2n}G^2(r) > 0, \quad r \in (R_2, R_1).$$

From (4), one has

$$\begin{aligned} F^2(r)r^2 &= r^{2-2n} \left(\int_{R_2}^r f(\rho) \rho^{n-1} d\rho \right)^2 \\ &\leq r^{2-2n} \left(\int_{R_2}^r |f(\rho)| \rho^{n-1} d\rho \right)^2 \\ &= r^{2-2n} \Gamma^2(n/2) / (4\pi^n) \|f\|_{L^1(\Omega)}^2 \\ &< (R_2/r)^{2n-2} 8\lambda^3\nu^2/27 \\ &< 8\lambda^3\nu^2/27. \end{aligned}$$

- According to the definition of ζ , one knows immediately that for $\bar{\zeta}_1 > 0$,

$$\delta_\phi^2 I(\bar{u}_1) \geq 0, \quad \delta_\psi^2 I_d(\bar{\zeta}_1) \leq 0.$$

- Since $\bar{\zeta}_3 < -2/3\nu\lambda$, then $\delta_\phi^2 I_d(\bar{\zeta}_3) \leq 0$ and $\lambda > 3/2|\nabla \bar{u}_3|^2$. In this case,

$$\begin{aligned} \delta_\phi^2 I(\bar{u}_3) &\leq \nu \int_{\Omega} \left\{ |\nabla \bar{u}_3|^2 |\nabla \phi|^2 + \left(1/2 |\nabla \bar{u}_3|^2 - \lambda \right) |\nabla \phi|^2 \right\} dx \\ &= \nu \int_{\Omega} \left(3/2 |\nabla \bar{u}_3|^2 - \lambda \right) |\nabla \phi|^2 dx \leq 0. \end{aligned}$$

- Indeed, $-2\nu\lambda/3 < \bar{\zeta}_2 < 0$ indicates $\lambda \in (1/2|\nabla\bar{u}_2|^2, 3/2|\nabla\bar{u}_2|^2)$. In this case, $\delta_\psi^2 I_d(\bar{\zeta}_2) \geq 0$. As for the 1D case, $\delta_\phi^2 I(\bar{u}_2) \geq 0$, which induces that \bar{u}_2 is a local minimizer in 1D. But for the higher dimensional case $n \geq 2$, \bar{u}_2 is not necessarily a local minimizer, which is in direct contrast to the 1D case.

In the final analysis, together with the fact $F \in C^1[R_2, R_1]$, definition of E , (17) and (18), we have

$$\lim_{\rho \rightarrow R_2^+} F(\rho)\rho/E_i^{-1}(F^2(\rho)\rho^2) < \infty, \quad i = 1, 2, 3,$$

and

$$\lim_{\rho \rightarrow R_1^-} F(\rho)\rho/E_i^{-1}(F^2(\rho)\rho^2) < \infty, \quad i = 1, 2, 3,$$

which indicate $\bar{u}_i \in C(\bar{\Omega})$, $i = 1, 2, 3$. And the proof of Theorem 1.1 is concluded.

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